CLAIMS

We Claim:

[c01] A method for reducing the time required for analyzing at least one sample for a parameter of interest which comprises collecting analytical data from a sample using a predetermined integration time T_a and applying mathematical transform analysis on the data, wherein the mathematical transform analysis is performed using conditions designed to achieve a pre-determined signal quality response function value comprising the value obtained when samples are analyzed without mathematical transform analysis using integration time T_b, wherein T_b is greater than T_a.

[c02] The method of claim 1, wherein the mathematical transform analysis comprises multivariate analysis.

[c03] The method of claim 2, wherein the multivariate analysis comprises neural networks analysis, principal components analysis, partial least squares analysis, linear multivariate analysis, or nonlinear multivariate analysis.

[c04] The method of claim 1, wherein the mathematical transform analysis comprises discrete transform analysis.

[c05] The method of claim 1, wherein the mathematical transform analysis comprises continuous transform analysis.

[c06] The method of claim 1, wherein the mathematical transform analysis comprises time averaging analysis, smoothing analysis or Savitsky-Golay analysis.

[c07] The method of claim 1, wherein the mathematical transform analysis comprises Fourier transform, Gabor transform, or Hadamard transform.

[c08] The method of claim 1, wherein the mathematical transform analysis comprises wavelet transform.

[c09] The method of claim 8, wherein the wavelet transform analysis comprises a wavelet de-noising algorithm.

[c10] The method of claim 9, wherein the wavelet de-noising algorithm comprises wavelet filters.

[c11] The method of claim 9, wherein the wavelet de-noising algorithm comprises a threshold/shrinkage method.

[c12] The method of claim 1, wherein parameters of the mathematical transform are determined during the course of analysis.

[c13] The method of claim 1, wherein the pre-determined signal quality response function comprises one or more measured signal parameters.

[c14] The method of claim 13, wherein at least one of the measured signal parameters comprises signal resolution.

[c15] The method of claim 13, wherein at least one of the measured signal parameters comprises peak shift.

[c16] The method of claim 13, wherein at least one of the measured signal parameters comprises signal distortion.

[c17] The method of claim 13, wherein at least one of the measured signal parameters comprises a signal-to-noise ratio.

[c18] The method of claim 17, wherein the signal-to-noise ratio ranges from 1 to 10,000.

[c19] The method of claim 17, wherein the signal-to-noise ratio ranges from 2 to 5,000.

[c20] The method of claim 17, wherein the signal-to-noise ratio ranges from 3 to 1,000.

[c21] The method of claim 1, wherein the analytical data comprises a first-order array.

[c22] The method of claim 1, wherein the analytical data comprises a second-order or higher array.

[c23] The method of claim 1, wherein the analytical data comprise spectroscopic, imaging, sensor, or scanning data.

[c24] The method of claim 23, wherein the data further comprise measurements made using Raman, luminescence, ultraviolet-visible molecular absorbance, atomic absorbance, infra-red, near infrared, surface plasmon resonance, mass spectrometry, X-ray, nuclear magnetic resonance, refractometry, interferometry, scattering, inductively coupled plasma, atomic force microscopy, scanning tunneling microscopy, microwave evanescent wave microscopy, near-field scanning optical microscopy, atomic fluorescence, laser-induced breakdown spectroscopy, Auger electron spectroscopy, X-ray photoelectron spectroscopy, ultrasonic spectroscopy, dielectric spectroscopy, microwave spectroscopy, resonance-enhanced multiphoton ionization, or combinations thereof.

[c25] The method of claim 23, wherein the data further comprise measurements made using photon probe microscopy, electron probe microscopy, ion probe microscopy, field probe microscopy, or scanning probe microscopy techniques.

[c26] The method of claim 1, wherein analytical data is provided using techniques relying on collection of electromagnetic radiation in the range from 0.05 Angstroms to 500 millimeters (mm).

[c27] The method of claim 1, wherein the sample comprises inorganic material, organic material, polymeric material, biological material, or combinations thereof.

[c28] The method of claim 1, wherein the parameter of interest is determined in the range from a single molecule to up to 100% of the sample.

[c29] Computer readable media comprising software code for performing the method of claim 1.

[c30] A method for reducing the time required for analyzing at least one sample for a parameter of interest which comprises:

selecting a pre-determined signal quality response function;

selecting a pre-determined integration time T_a;

collecting analytical data from a sample with integration time T_a;

applying a screening rate accelerator toolbox comprising mathematical transform analysis to the data, wherein the mathematical transform analysis is performed using conditions designed to achieve a pre-determined signal quality response function value comprising the value obtained when samples are analyzed without mathematical transform analysis using integration time T_b, wherein T_b is greater than T_a; and

analyzing the data processed by the screening rate accelerator toolbox for the parameter of interest.

[c31] The method of claim 30, wherein the mathematical transform analysis comprises multivariate analysis.

[c32] The method of claim 31, wherein the multivariate analysis comprises neural networks analysis, principal components analysis, partial least squares analysis, linear multivariate analysis, or nonlinear multivariate analysis.

[c33] The method of claim 30, wherein the mathematical transform analysis comprises discrete transform analysis.

[c34] The method of claim 30, wherein the mathematical transform analysis comprises continuous transform analysis.

[c35] The method of claim 30, wherein the mathematical analysis comprises time averaging analysis, smoothing analysis or Savitsky-Golay analysis.

[c36] The method of claim 30, wherein the mathematical transform analysis comprises Fourier transform, Gabor transform, or Hadamard transform.

[c37] The method of claim 30, wherein the mathematical transform analysis comprises wavelet transform.

[c38] The method of claim 37, wherein the wavelet transform analysis comprises a wavelet de-noising algorithm.

[c39] The method of claim 38, wherein the wavelet de-noising algorithm comprises wavelet filters.

[c40] The method of claim 38, wherein the wavelet de-noising algorithm comprises a threshold/shrinkage method.

[c41] The method of claim 30, wherein parameters of the mathematical transform are determined during the course of analysis.

[c42] The method of claim 30, further comprising determining whether the analytical data collected from the sample with integration time T_a satisfies the pre-determined signal quality response function value prior to applying the screening rate accelerator toolbox and applying the screening rate accelerator toolbox if the collected data does not satisfy the pre-determined signal quality response function value, but not if the collected data does satisfy the pre-determined signal quality response function value.

[c43] The method of claim 30, further comprising the steps of:

determining whether the data processed by the screening rate accelerator toolbox satisfies the pre-determined signal quality response function value; and

if the processed data does not satisfy the pre-determined signal quality response value, re-applying the screening rate accelerator toolbox using a mathematical transform analysis different from the analysis previously applied until the data processed using the screen rate accelerator toolbox either satisfies the pre-determined signal quality response function value or comprises an optimized signal quality response function value.

[c44] The method of claim 43, further comprising repeating the method with a new, larger value for T_a if the data which is optimized using the screening rate accelerator toolbox does not satisfy the pre-determined signal quality response function value.

[c45] The method of claim 30, wherein if the collected data does not require application of the screening rate accelerator toolbox to satisfy a pre-determined signal quality response function value, a shorter pre-determined integration time T_a is selected, and the method is performed using the new value for T_a.

[c46] The method of claim 30, wherein the preset signal quality response function comprises one or more measured signal parameters.

[c47] The method of claim 46, wherein at least one of the measured signal parameters comprises signal resolution.

[c48] The method of claim 46, wherein at least one of the measured signal parameters comprises peak shift.

[c49] The method of claim 46, wherein at least one of the measured signal parameters comprises signal distortion.

[c50] The method of claim 46, wherein at least one of the measured signal parameters comprises a signal-to-noise ratio.

[c51] The method of claim 50, wherein the signal to noise ratio ranges from 1 to about 10,000.

[c52] The method of claim 50, wherein the signal to noise ratio ranges from 2 to 5,000.

[c53] The method of claim 50, wherein the signal to noise ratio ranges from 3 to 1,000.

[c54] The method of claim 30, wherein the relative improvement in signal integration time (T_b /T_a) ranges from about 1.5 to 1,000 fold.

[c55] The method of claim 30, wherein the relative improvement in signal integration time (T_b /T_a) ranges from about 1.5 to 500 fold.

[c56] The method of claim 30, wherein the relative improvement in signal integration time (T_b /T_a) ranges from about 1.5 to 200 fold.

[c57] The method of claim 30, wherein the analytical data comprises a first-order array.

[c58] The method of claim 30, wherein the analytical data comprises a multi-order array.

[c59] The method of claim 30, further comprising simultaneous evaluation of each individual sample in an array of samples.

[c60] The method of claim 30, wherein the analytical data comprise spectroscopic, imaging, sensor, or scanning data.

[c61] The method of claim 60, wherein the data further comprise measurements made using Raman, luminescence, ultraviolet-visible molecular absorbance, atomic absorbance, infra-red, near infrared, surface plasmon resonance, mass spectrometry, X-ray, nuclear magnetic resonance, refractometry, interferometry, scattering, inductively coupled plasma, atomic force microscopy, scanning tunneling microscopy, microwave evanescent wave microscopy, near-field scanning optical microscopy, atomic fluorescence, laser-induced breakdown spectroscopy, Auger electron spectroscopy, X-ray photoelectron spectroscopy, ultrasonic spectroscopy, dielectric spectroscopy, microwave spectroscopy, resonance-enhanced multiphoton ionization, or combinations thereof.

[c62] The method of claim 60, wherein the data further comprise measurements made using photon probe microscopy, electron probe microscopy, ion probe microscopy, field probe microscopy, or scanning probe microscopy techniques.

[c63] The method of claim 30, wherein analytical data is provided using techniques relying on collection of electromagnetic radiation in the range from 0.05 Angstroms to 500 millimeters (mm).

[c64] The method of claim 30, wherein the sample comprises inorganic material, organic material, polymeric material, biological material, or combinations thereof.

[c65] The method of claim 30, wherein the parameter of interest ranges from a single molecule to up to 100% of the sample.

[c66] The method of claim 30, wherein the sample comprises polycarbonate.

[c67] Computer readable media comprising software code for performing the method of claim 30.

[c68] An apparatus for analyzing at least one sample for a parameter of interest using a pre-determined signal quality response function which comprises:

a collecting system for collecting analytical data comprising the parameter of interest from a sample;

a processing system for processing the analytical data;

a screening rate accelerator toolbox for applying mathematical transform analysis to the data;

a data analysis system for determining whether the data processed by the screening rate accelerator toolbox satisfies a pre-determined signal quality response function value; and

a statistical toolbox for analyzing the processed data for the parameter of interest.

[c69] The apparatus of claim 68, wherein the mathematical transform analysis comprises multivariate analysis.

[c70] The apparatus of claim 69, wherein the multivariate analysis comprises neural networks analysis, principal components analysis, partial least squares analysis, linear multivariate analysis, or nonlinear multivariate analysis.

[c71] The apparatus of claim 68, wherein the mathematical transform analysis comprises discrete transform analysis.

[c72] The apparatus of claim 68, wherein the mathematical transform analysis comprises continuous transform analysis.

[c73] The apparatus of claim 68, wherein the mathematical analysis comprises time averaging analysis, smoothing analysis or Savitsky-Golay analysis.

[c74] The apparatus of claim 68, wherein the mathematical transform analysis comprises Fourier transform, Gabor transform, or Hadamard transform.

[c75] The apparatus of claim 68, wherein the mathematical transform analysis comprises wavelet transform.

[c76] The apparatus of claim 68, wherein the parameters of the mathematical transform are determined during the course of analysis.

[c77] The apparatus of claim 68, wherein the preset signal quality response function comprises one or more measured signal parameters.

[c78] The apparatus of claim 77, wherein at least one of the measured signal parameters comprises a signal-to-noise ratio.

[c79] The apparatus of claim 77, wherein at least one of the measured signal parameters comprises signal resolution.

[c80] The apparatus of claim 77, wherein at least one of the measured signal parameters comprises signal distortion.

[c81] The apparatus of claim 77, wherein at least one of the measured signal parameters comprise peak shift.

[c82] The apparatus of claim 68, further comprising at least one energy source for interacting with a sample.

[c83] The apparatus of claim 82, wherein the energy source comprises a light source, an ion source, or a radiation source.

[c84] The apparatus of claim 68, wherein the collecting system comprises an optical spectrometer, an ion spectrometer, a mass detector, or an imaging camera.

[c85] The apparatus of claim 68, wherein the analytical data comprises a first-order array.

[c86] The apparatus of claim 68, wherein the analytical data comprises a multi-order array.

[c87] The apparatus of claim 68, further comprising simultaneous evaluation of each individual sample in an array of samples.

[c88] The apparatus of claim 68, wherein the analytical data comprise spectroscopic, imaging, scanning, and sensor data.

[c89] The apparatus of claim 88, wherein the data further comprise measurements made using Raman, luminescence, ultraviolet-visible molecular absorbance, atomic absorbance, infra-red, near infrared, surface plasmon resonance, mass spectrometry, X-ray, nuclear magnetic resonance, refractometry, interferometry, scattering, inductively coupled plasma, atomic force microscopy, scanning tunneling microscopy, microwave evanescent wave microscopy, near-field scanning optical microscopy, atomic fluorescence, laser-induced breakdown, Auger electron spectroscopy, X-ray photoelectron spectroscopy, ultrasonic spectroscopy, dielectric spectroscopy, microwave spectroscopy, resonance-enhanced multiphoton ionization, or combinations thereof.

[c90] The apparatus of claim 88, wherein the data further comprise measurements made using photon probe microscopy, electron probe microscopy, ion probe microscopy, field probe microscopy, or scanning probe microscopy techniques.

[c91] The apparatus of claim 68, wherein analytical data is provided using techniques relying on collection of electromagnetic radiation in the range from 0.05 Angstroms to 500 millimeters (mm).

[c92] The apparatus of claim 68, further comprising computer readable media comprising software code.